Trifluoromethanesulfonic acid

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 90.2 °C

Global applicability domain: Inside

Local applicability domain index: 2.93e-01

Confidence level: 6.09e-01

Nearest Neighbors from the Training Set

Image not found
2,3,4,5,6-Pentafluorobenzamide
Measured: 147
Predicted: 132

Image not found
Acetic acid, chlorodifluoro-
Measured: 25.0
Predicted: 33.2

Image not found
Butanedioic acid, 2,2,3,3-
tetrafluoro-
Measured: 119
Predicted: 116

Image not found
2-(Trifluoromethyl)acrylic acid
Measured: 51.5
Predicted: 57.7

Image not found
(Pentafluorophenoxy)acetic acid
Measured: 109
Predicted: 110